Researchers stitch defects into the world's thinnest semiconductor

May 22 2013

(Phys.org) —In pioneering new research at Columbia University, scientists have grown high-quality crystals of molybdenum disulfide (MoS2), the world's thinnest semiconductor, and studied how these crystals stitch together at the atomic scale to form continuous sheets. Through beautiful images of strikingly symmetric stars and triangles hundreds of microns across, they have uncovered key insights into the optical and electronic properties of this new material, which can be either conducting or insulating to form the basic "on-off switch" for all digital electronics. The study is published in the May 5, 2013, issue of *Nature Materials*.

"Our research is the first to systematically examine what kinds of defects result from these large growths, and to investigate how those defects change its properties," says James Hone, professor of mechanical engineering at Columbia Engineering, who led the study. "Our results will help develop ways to use this new material in atomically thin electronics that will become integral components of a whole new generation of revolutionary products such as flexible solar cells that conform to the body of a car."

This multidisciplinary collaboration by the Energy Frontier Research Center at Columbia University with Cornell University's Kavli Institute for Nanoscale Science focused on molybdenum disulfide because of its potential to create anything from highly efficient, flexible solar cells to conformable touch displays. Earlier work from Columbia demonstrated that monolayer MoS2 has an electronic structure distinct from the bulk form, and the researchers are excited about exploring other atomically thin metal dichalcogenides, which should have equally interesting properties. MoS2 is in a class of materials called transition metal dichalcogenides, which can be metals, semiconductors, dielectrics, and even superconductors.

"This material is the newest in a growing family of two-dimensional crystals," says Arend van der Zande, a research fellow at the Columbia Energy Frontier Research Center and one of the paper's three lead authors. "Graphene, a single sheet of carbon atoms, is the thinnest electrical conductor we know. With the addition of the monolayer molybdenum disulfide and other metal dichalcogenides, we have all the building blocks for modern electronics that must be created in atomically thin form. For example, we can now imagine sandwiching two different monolayer transition metal dichalcogenides between layers of graphene to make solar cells that are only eight atoms thick—20 thousand times smaller than a human hair!"

Until last year, the majority of experiments studying MoS2 were done by a process called mechanical exfoliation, which only produces samples just a few micrometers in size. "While these tiny specimens are fine for scientific studies," notes Daniel Chenet, a PhD in Hone's lab and another lead author, "they are much too small for use in any technological application. Figuring out how to grow these materials on a large scale is critical."

To study the material, the researchers refined an existing technique to grow large, symmetric crystals up to 100 microns across, but only three atoms thick. "If we could expand one of these crystals to the thickness of a sheet of plastic wrap, it would be large enough to cover a football field—and it would not have any misaligned atoms," says Pinshane Huang, a PhD student in the David Muller lab at Cornell and the paper's third lead author.

For use in many applications, these crystals need to be joined together into continuous sheets like patches on a quilt. The connections between the crystals, called grain boundaries, can be as important as the crystals themselves in determining the material's performance on a large scale. "The grain boundaries become important in any technology," says Hone. "Say, for example, we want to make a solar cell. Now we need to have meters of this material, not micrometers, and that means that there will be thousands of grain boundaries. We need to understand what they do so we can control them."

The team used atomic-resolution electron microscopy to examine the grain boundaries of this material, and saw lines of misaligned atoms. Once they knew where to find the grain boundaries, and what they looked like, the team could study the effect of a single grain boundary on the properties of the MoS2. To do this, they built tiny transistors, the most basic component in all of electronics, out of the crystals and saw that the single, defective line of atoms at the grain boundaries could drastically change the key electronic and optical properties of the MoS2.

"We've made a lot of progress in controlling the growth of this new 'wonder' nanomaterial and are now developing techniques to integrate it into many new technologies," Hone adds. "We're only just beginning to scratch the surface of what we can make with these materials and what their properties are. For instance, we can easily remove this material from the growth substrate and transfer it on to any arbitrary surface, which enables us to integrate it into large-scale, flexible electronics and solar cells."

The crystal synthesis, optical measurements, electronic measurements, and theory were all performed by research groups at Columbia Engineering. The growth and electrical measurements were made by the Hone lab in mechanical engineering; the optical measurements were carried out in the Tony Heinz lab in physics. The structural modeling and electronic structure calculations were performed by the David Reichman lab in chemistry. The electron microscopy was performed by atomic imaging experts in the David Muller lab at Cornell University's School of Applied and Engineering Physics, and the Kavli Institute at Cornell for Nanoscale Science.

Provided by Columbia University

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